

pK_a measurements for the SAMPL6 prediction challenge for a set of kinase inhibitor-like fragments

Mehtap Işık^{1,2}, Dorothy Levorse³, Ariën S. Rustenburg^{1,4}, Ikenna E. Ndukwe⁵, Heather Wang⁶, Xiao Wang⁵, Mikhail Reibarkh⁵, Gary E. Martin⁵, Alexey A. Makarov⁶, David L. Mobley⁷, Timothy Rhodes^{3*}, John D. Chodera^{1*,6}

¹ Computational and Systems Biology Program, Sloan Kettering Institute, Memorial Sloan Kettering Cancer Center, New York, NY 10065, United States

² Tri-Institutional PhD Program in Chemical Biology, Weill Cornell Graduate School of Medical Sciences, Cornell University, New York, NY 10065, United States

³ Pharmaceutical Sciences, MRL, Merck & Co., Inc., 126 East Lincoln Avenue, Rahway, New Jersey 07065, United States

⁴ Graduate Program in Physiology, Biophysics, and Systems Biology, Weill Cornell Medical College, New York, NY 10065, United States

⁵ Process and Analytical Research and Development, Merck & Co., Inc., Rahway, NJ 07065, United States

⁶ Analytical Research and Development, Merck & Co., Inc., Rahway, NJ 07065, United States

⁷ Department of Pharmaceutical Sciences and Department of Chemistry, University of California, Irvine, Irvine, California 92697, United States

*For correspondence:

john.chodera@choderalab.org (JDC)

timothy_rhodes@merck.com (TR)

SUPPLEMENTARY INFORMATION